Theoretical Studies on Novel Physical Properties Arising from Many-Body Interaction

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Professional Employment
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2011 Best Poster Award in ISSS-6 Internal Symposium on Surface Science
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Quantum many-body interaction is a source of novel physical properties in the condensed matters. In our group, we develop theoretical methods by combining quantum field theory and density functional theory, and carry out collaborative research with experimental groups. As specific targets, we focus on magnetism in nanostructure and energy dissipation.

For magnetism in nanostructure, we are interested in the Kondo effect and spin–orbit interaction. The Kondo effect arises from the interaction between the localized spin and conduction electrons, which forms a characteristic many-body state so called the Kondo singlet state. The spin–orbit interaction originating from relativistic effect constrains the direction of magnetic moment to specific direction. We investigate the possibility of novel physical phenomena induced by these interactions in the nanostructure and molecules on surfaces.

For energy dissipation, we focus on the effect of electron–phonon interaction. The electron–phonon interaction is one of the most fundamental interactions in the condensed matter physics, and the quantitative evaluation in realistic materials is highly demanding. We adopt the ab-initio calculation to analyze the signal of electron–phonon coupling in surface spectroscopy and thermal properties in various kind of solids.

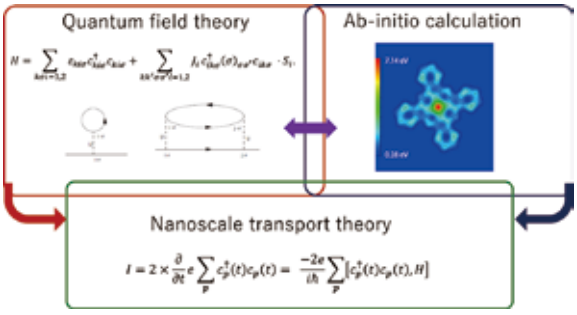

Figure 1. Schematic image of the theoretical method developed in our group.

Selected Publications

- E. Minamitani, N. Tsukahara, D. Matsunaka, Y. Kim, N. Takagi and M. Kawai, "Symmetry-Driven Novel Kondo Effect in a Molecule," *Phys. Rev. Lett.* **109**, 086602 (2012).
- E. Minamitani, R. Arafune, N. Tsukahara, Y. Ohda, S. Watanabe, M. Kawai, H. Ueba and N. Takagi, "Surface Phonon Excitation on Clean Metal Surfaces in Scanning Tunneling Microscopy," *Phys. Rev. B* **93**, 085411 (2016).
- E. Minamitani, N. Takagi and S. Watanabe, "Model Hamiltonian Approach to the Magnetic Anisotropy of Iron Phthalocyanine at Solid Surfaces," *Phys. Rev. B* **94**, 205402 (2016).
- R. Hiraoka, E. Minamitani, R. Arafune, N. Tsukahara, S. Watanabe, M. Kawai and N. Takagi, "Single-Molecule Quantum Dot as a Kondo Simulator," *Nat. Commun.* **8**, 16012 (2017).
- E. Minamitani, R. Arafune, T. Frederiksen, T. Suzuki, S. M. F. Shahed, T. Kobayashi, N. Endo, H. Fukidome, S. Watanabe and T. Komeda, "Atomic-Scale Characterization of the Interfacial Phonon in Graphene/SiC," *Phys. Rev. B* **96**, 155431 (2017).

1. Simulating Lattice Thermal Conductivity in Semiconducting Materials Using High-Dimensional Neural Network Potential

Heat generation in semiconducting materials has become a critical problem in modern nanoscale electronics. To design semiconductor materials with better thermal manageability, efficient methods for theoretical simulation of the thermal conductivity are required.

The main carrier of heat in semiconductors is the phonon, which is a quantum of lattice vibration. Current methods of simulating lattice thermal conductivity require accurate prediction of the interatomic force in the solid. Density functional theory (DFT) calculation is one of the most well-established techniques for accurate force prediction, including the effect of changes in the electronic state with atomic displacement. However, the high computational cost limits the application of DFT calculation in thermal conductivity simulations.

We focus on the application of machine learning techniques for thermal conductivity simulations.[1] Among various machine learning techniques, we chose the high-dimensional neural network potential (HDNNP) developed by Behler *et al.*[2,3] HDNNP can describe the relation between the total energy of a system and its atomic arrangement. The force acting on atoms can also be described by the HDNNP as shown in several previous studies, however, the accuracy of the prediction is limited. We showed that much higher accuracy can be obtained by training HDNNP parameters with a focus on force fitting. We chose crystalline Si and GaN as representative semiconducting materials with one and two atom types, respectively.

Figure 2 shows the compare the forces in the Si and GaN systems predicted by DFT and HDNNP. The root mean square error (RMSE) between force prediction from HDNNP and DFT calculation results was 25.5 meV/Å for Si and 37.8 meV/Å for GaN.

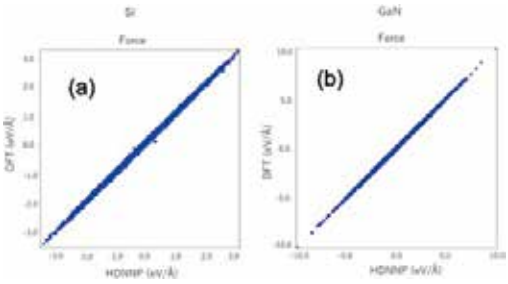

Figure 2. Comparison of interatomic forces in (a) Si and (b) GaN bulk crystals obtained by HDNNP and DFT calculations.

The phonon dispersion curves obtained using HDNNP agree well with the DFT calculation results and previous reports for both Si and GaN,[4,5] as shown in Figure 3. Then, we simulated the lattice thermal conductivity based on ALD by combining HDNNP and phono3py package.[6] Figure 4 shows a comparison of the temperature dependence of the thermal conductivity obtained from the force predictions of HDNNP and VASP calculations. The deviation from the DFT calculation results is within 1% at 200 to 500 K for Si and within 5.4% from 200 to 1000 K for GaN.

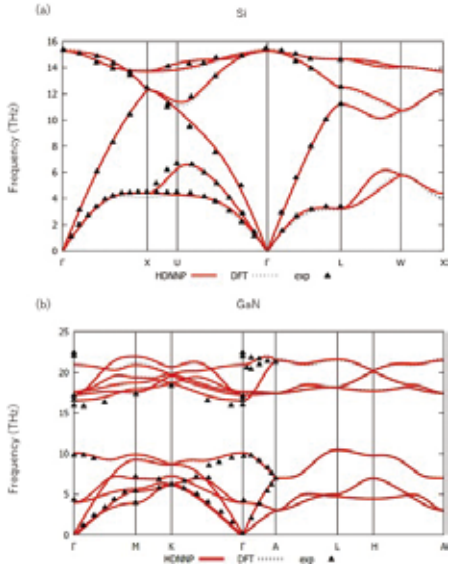

Figure 3. Comparison of phonon dispersions in (a) Si and (b) GaN obtained by HDNNP and DFT calculations. The experimental data for comparison were obtained from Ref. 4 for Si and Ref. 5 for GaN.

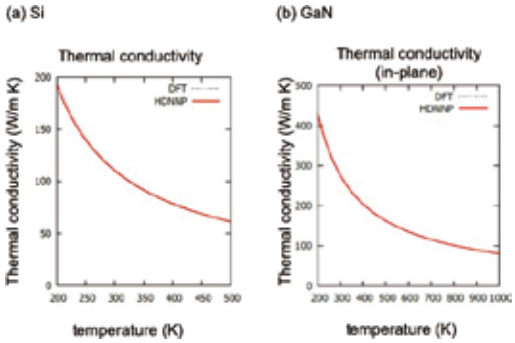

Figure 4. Comparison of thermal conductivities in (a) Si, (b) along the in-plane (100) direction in GaN obtained by HDNNP and DFT calculations.

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Award

MINAMITANI, Emi; The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology The Young Scientists' Prize (2019).